STUDY OF BOUND AND SCATTERING STATES OF THREE–NUCLEON SYSTEMS

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Abstract. A variational technique to describe the ground and scattering states below the break–up threshold for a three-nucleon system is developed. The method consists in expanding the wave function in terms of correlated Harmonic Hyperspherical functions suitable to handle the large repulsion contained in the nuclear potential at short distances; three body forces have also been considered. The inclusion of the pp Coulomb repulsion in the p–d processes does not cause any particular problem, since no partial wave decomposition of the interaction is performed. Accurate numerical results are given for ground state properties and scattering lenghts, phase shifts and mixing parameters at three different energies of the incident nucleon. The agreement with other available results and with experimental analyses is higlly satisfactory.

1. Introduction

A sophisticated variational technique to describe the bound state of a three–nucleon system has been developed by the authors in ref.[1]. The wave function is expanded in channels, as in the Faddeev technique, and for each channel, the radial amplitude is, in turn, expanded in terms of correlated functions, constituting the Pair correlated Hyperspherical Harmonic (PHH) basis; such a basis results to be well suited to carefully take into account the correlations induced by the large repulsive terms of the nucleon–nucleon (NN) potential. This technique was applied in [1] to calculate the bound state w.f. of the triton, with the Argonne 14 (AV14) model of NN interaction [2], with results in complete agreement with those given by the best available techniques [3–5].

It is well known that local NN pairwise potentials, as determined by fitting the two nucleon scattering data, do not give the correct binding energies of systems with A$\geq$ 3. If such potentials provide a very precise fit to the data (χ^2 per datum

≈ 1), their predictions for the triton binding energy nearly coincide [6] among themselves; nevertheless, appreciable differences continue to exist with the corresponding experimental values. The lack of binding in the three–nucleon systems with these models, has been attributed to different possible causes, such as relativistic corrections, non–local effects and three body interaction (TBI) terms in the Hamiltonian. Charge symmetry breaking (CSB) terms are also important to understand the mass difference between ^{3}H and ^{3}He, but give a minor contribution to the total energy. Of course, all these effects are not independent from each other and their correct description is a difficult task.

One of the most important aims in few-nucleon theory is testing realistic NN potentials, not only in the bound states, but in continuum states too, mainly in those related to the A=3 systems. As a matter of fact, a series of theoretical investigations has been devoted to the study of the p–d and n–d elastic scattering and break–up reactions. The general status of the field is satisfactory [7] and an overall agreement between theory and experiments has been reached. Among the possible improvements, here we shall be interested in a correct treatment of the Coulomb forces and in a detailed comparison of theoretical and experimental results. To this end we have extended the method of ref.[1] to describe N–d scattering processes and, in this paper, our attention will be devoted to the study of states below the deuteron break–up treshold. The break–up reactions will be the object of a subsequent paper.

We are here particurarly interested to calculate scattering lengths and phase shifts for the various N–d elastic scattering channels, to be compared with the existing experimental analysis [8]. However, such quantities are strictly related to the ground state energy (for example, the doublet scattering lenght and the binding energy lie on the so–called Philips line [9]). As already atated, the AV14 interaction alone, as considered in ref.[1], is not adequate and for this reason, we have included TBI terms in the the Hamiltonian. These terms have been proposed to take into account all the important two pion exchange effects, in an approximate but quantitative way. We will consider in this paper the so–called Tucson–Melbourne (TM) [10] and Brazil (BR) [11] three–body potentials.

One important aspect of the present calculations is the extension of the variational method to scattering states. The Rayleigh–Ritz variational principle has a long tradition in nuclear physics and it has been largely used, starting from the first attemps to investigate the bound state of few–nucleon systems. On the other hand, a few calculations exist for scattering states and, among them, those using variational techniques, as the Kohn–Hultén principle, are scarce. The reason is related to the difficulty of obtaining accuracies comparable with those of bound state calculations.

In recent times, accurate variational techniques were developed to solve the three– [1,3] and four–nucleon [12] problems, showing a fast convergence in the number of channels when compared with the Faddeev techniques. It is natural to ask

whether the situation would be similar in the case of scattering states. This is one more motivation for the present work.

The paper is organized in the following way: in section 2 the construction of the trinucleon bound state w.f. in terms of the PHH basis functions is worked out and the resulting equations are solved with the inclusion of TBI terms; in the next section the method is extended to describe N–d scattering states below the deuteron break–up threshold; the basic equations which allow to determine the w.f and the reactance matrix $\Re$ are obtained in the frame of the Kohn variational principle; the numerical procedure used to solve those equations is shortly outlined in sections 2 and 4 and, in the latter the results obtained for the scattering lengths and phase shifts are given. Finally, the merits of the approach are discussed in the last section, together with its possible extension to other problems.

2. The three–nucleon bound state.

The three–nucleon Hamiltonian is taken to have the form

$$H = T + \sum_{i<j} V(i,j) + \sum_{i<j<k} W(i,j,k) \ , \tag{2.1}$$

where T is the non relativistic total kinetic energy operator and the two– and three–body interactions, V and W, are explicitely included. The Coulomb p–p repulsion, if it is present, is contained in the two–body potential; moreover, the three particles are assumed to have the same mass ($\hbar^2/M = 41.47$ MeV fm^2 throughout the paper). Let us introduce, in the center of mass (c.m.) frame, the following set of Jacobi coordinates (i, j, $k = 1$, 2, 3 cyclic)

$$\mathbf{x}_i = (\mathbf{r}_j - \mathbf{r}_k), \quad \mathbf{y}_i = \frac{2}{\sqrt{3}}(\mathbf{r}_j + \mathbf{r}_k - 2\mathbf{r}_i) \ . \tag{2.2}$$

The w.f. of the system is written as a sum of three Faddeev amplitudes,

$$\Psi = \psi(\mathbf{x}_i, \mathbf{y}_i) + \psi(\mathbf{x}_j, \mathbf{y}_j) + \psi(\mathbf{x}_k, \mathbf{y}_k) \ . \tag{2.3}$$

In the above equation, each amplitude corresponds to a total angular momentum JJ_z and total isospin TT_z, therefore, if we use the L–S coupling, it can be written in the form

$$\psi(\mathbf{x}_i, \mathbf{y}_i) = \sum_{\alpha=1}^{N_c} \Phi_\alpha(x_i, y_i) \mathcal{Y}_\alpha(jk, i) \tag{2.4a}$$

$$\mathcal{Y}_\alpha(jk,i) = \Big\{ \big[Y_{\ell_\alpha}(\hat{x}_i) Y_{L_\alpha}(\hat{y}_i) \big]_{\Lambda_\alpha} \big[s_\alpha^{jk} s_\alpha^i \big]_{S_\alpha} \Big\}_{JJ_z} \big[t_\alpha^{jk} t_\alpha^i \big]_{TT_z} \ , \tag{2.4b}$$

where x_i, y_i are the moduli of the Jacobi coordinates. Each α– channel is specified by the angular momenta ℓ_α, L_α coupled to give Λ_α, and by the spin (isospin) s_α^{jk} (t_α^{jk}) and s_α^i (t_α^i) of the pair j, k and the third particle i, coupled to give S_α (T). The number N_c of channels taken into account to construct the w.f. can be increased until convergence is reached. The antisymmetrization of the w.f. Ψ requires $\ell_\alpha + s_\alpha^{jk} + t_\alpha^{jk}$ to be odd; in addition $\ell_\alpha + L_\alpha$ must be even for positive parity states and odd for the negative ones.

The ground state of the three–nucleon system has positive parity and $J = 1/2$, $T = 1/2$ (the inclusion of the Coulomb potential gives a small $T = 3/2$ contribution, disregarded in the present work, as well as other charge symmetry breaking terms in the Hamiltonian). The channels allowed by such conditions are easily obtained and ordered of increasing angular momenta values; for example, they are 10, 18 and 26 for $\ell_\alpha + L_\alpha \leq 2$, $\ell_\alpha + L_\alpha \leq 4$ and $\ell_\alpha + L_\alpha \leq 6$, respectively.

Let us introduce, in place of the coordinates x_i, y_i, the hyperspherical coordinates defined by:

$$x_i = \rho \cos\phi_i \ , \quad y_i = \rho \sin\phi_i \ , \tag{2.5}$$

where ρ is the hyperradius. The radial dependence of each α–amplitude in the w.f. (2.4a) is now expanded in terms of the PHH basis functions in the following way:

$$\Phi_\alpha(x_i, y_i) = \rho^{\ell_\alpha + L_\alpha} f_\alpha(x_i) \Big[\sum_{K=K_0}^{K_\alpha} u_K^\alpha(\rho) \ {}^{(2)}P_K^{\ell_\alpha, L_\alpha}(\phi_i) \Big] \ , \tag{2.6}$$

where the hyperspherical polynomials are given by [13]

$${}^{(2)}P_K^{\ell_\alpha, L_\alpha}(\phi_i) = N_n^{\ell_\alpha, L_\alpha} (\sin\phi_i)^{L_\alpha} (\cos\phi_i)^{\ell_\alpha} P_n^{L_\alpha + 1/2, \ell_\alpha + 1/2}(\cos 2\phi_i) \ , \tag{2.7}$$

$N_n^{\ell_\alpha, L_\alpha}$ is a normalization factor and $P_n^{\alpha,\beta}$ is a Jacobi polynomial. The grand orbital quantum number is given by $K = \ell_\alpha + L_\alpha + 2n$, with n a non–negative integer. In eq.(2.6) $K_0 = \ell_\alpha + L_\alpha$ is the minimum grand orbital quantum number and K_α is the maximum selected value, so that the number of basis functions per channel is

$$M_\alpha = (K_\alpha - K_0)/2 + 1 \, , \tag{2.8}$$

corresponding to the maximum value of the index n plus one. When α goes to infinity, the expansion basis used in eq.(2.6) is obviously complete.

If the functions $f_\alpha(x_i)$ in eq.(2.6) are taken equal to one, the standard (uncorrelated) HH expansion is recovered. Such an expansion is well suited to describe the structure of the system in the case of soft interparticle potentials, where a rather small number of basis functions is sufficient to reproduce the w.f. within a reasonable accuracy [14]. However, for potentials containing a strong repulsion at small distances, the w.f. must be accurately determined for small interparticle

separation values and correspondingly the rate of convergence of the HH expansion results to be very slow [15]. The role of the correlation function $f_\alpha(x)$ in eq.(2.6) is therefore to fasten the convergence of the expansion by improving the description of the system when a pair of particles are close to each other. A simple procedure to determine the correlation functions is the one outlined in [1],where the functions $f_\alpha(r)$ are taken as the solutions of the following zero–energy Schroedinger equations

$$\sum_{\beta'}[T_{\beta,\beta'}(r) + V_{\beta,\beta'}(r) + \lambda_{\beta,\beta'}(r)]f_{\beta'}(r) = 0. \tag{2.9}$$

$T_{\beta,\beta'}$ and $V_{\beta,\beta'}$ are the kinetic and the potential energy operators,

$$\begin{aligned} T_{\beta,\beta'} &= -\frac{\hbar^2}{m}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\ell_\beta(\ell_\beta+1)}{r^2}\right]\delta_{\beta,\beta'}\,, \\ V_{\beta,\beta'} &= <\ell_\beta\ s^{jk}_{\beta'}\ t^{jk}_{\beta'}\ |V(jk)|\ell_\beta\ s^{jk}_{\beta}\ t^{jk}_{\beta}\ >\,, \end{aligned} \tag{2.10}$$

and $V(jk)$ is the NN potential; the term $\lambda_{\beta,\beta'}(r)$ in (2.9) is chosen of the simple form [1,16]

$$\lambda_{\beta,\beta'}(r) = \lambda^0_\beta \exp(-\gamma r)\delta_{\beta,\beta'} \tag{2.11}$$

and its role is to allow the function $f_\beta(r)$ to satisfy an appropriate healing condition. This can be achieved by taking γ as a trial parameter, whose precise value is not important (the choice $\gamma \approx .5\,\mathrm{fm}^{-1}$ is adequate [16]), and conveniently fixing the depth λ^0_β. As an example, in the case of an uncoupled channel we can require that

$$f_\beta(r) = 1, \quad \text{when} \quad r > R, \tag{2.12}$$

where R is large with respect to the range of the potential $V_{\beta,\beta'}(r)$. For coupled channels, the condition (2.12) is satisfied by the function associated with the lower angular momentum value, while the other function goes to zero when r becomes large.

The remaining problem is the determination of the hyperradial functions $u^\alpha_K(\rho)$ contained in eqs.(2.6); to this aim we will use the Rayleight–Ritz principle, requiring that the following condition to be satisfied

$$<\delta_u\Psi|H - E|\Psi>= 0\,, \tag{2.13}$$

where $\delta_u\Psi$ represents the change in the w.f. caused by an infinitesimal variation of the functions $u^\alpha_K(\rho)$. From the latter equation, it follows that

$$\rho^{\ell_\alpha+L_\alpha}\sum_i <f_\alpha(x_i)\ {}^{(2)}P^{\ell_\alpha,L_\alpha}_K(\phi_i)\mathcal{Y}_\alpha(jk,i)|H - E|\Psi>_\Omega= 0\,, \tag{2.14}$$

where the subscript Ω indicates that the integration over the hyperangles ϕ_i and the angles $\hat{x}_i, \hat{y}_i$ must be performed, and $d\Omega = \sin^2\phi_i \cos^2\phi_i \, d\phi_i d\hat{x}_i d\hat{y}_i$. From eq(2.14), after the evaluation of the spin–isospin traces and the angular integration, one obtains a set of second–order differential equations for the functions $u^{\alpha'}_{K'}(\rho)$ which can be written in the form [1]

$$\sum_{\alpha',K'} \Big[A^{\alpha,\alpha'}_{K,K'}(\rho) \frac{d^2}{d\rho^2} + B^{\alpha,\alpha'}_{K,K'}(\rho) \frac{d}{d\rho} + C^{\alpha,\alpha'}_{K,K'}(\rho) + \frac{m}{\hbar^2} E \; N^{\alpha,\alpha'}_{K,K'}(\rho) \Big] u^{\alpha'}_{K'}(\rho) = 0 \; , \quad (2.15)$$

with $\alpha' = 1, \ldots, N_c$ and $K' = K'_0, \ldots, K'_{\alpha'}$. A numerical technique for solving the set of eqs.(2.15) has been outlined in ref.[1]. An important point is to reduce as much as possible the number N of grid points $[\rho_1, \ldots, \rho_N]$ in the hyperradius, without losing accuracy in the solution. Due to the nature of the problem, the coefficients $X^{\alpha,\alpha'}_{K,K'}$ $(X = A, B, C, N)$, and correspondingly the solution, strongly vary only for small values of ρ; for this reason, a grid of the type $\rho_{k+1} - \rho_k = \chi(\rho_k - \rho_{k-1})$, where the step–length is increased by a constant factor, results to be a convenient choice. As a consequence, a new variable w is introduced with equally spaced grid values w_k and the corresponding ρ_k values can be obtained by the relation

$$w = \frac{h}{\ln \chi} \ln[1 + \frac{\rho}{h}(\chi - 1)] \quad (2.16)$$

with $h = \rho_2 - \rho_1$. For potentials without hard-core repulsion, as the ones considered here, we have $\rho_1 = w_1 = 0$, and the last grid point w_N can be chosen so that $\rho_N = \rho_{max}$ is about $20 \div 25$ fm for bound state calculations. The set of eqs.(2.15) can be re–written in terms of the variable w and the corresponding generalized eigenvalue problem then solved by standard procedures.

Another useful possibility is to introduce a new variable to map the infinite range of the hyperradius $[0, \infty]$ into the finite interval $[0, 1]$. The new variable is then transformed into the variable w which is used with a constant step grid. This is achieved by the following two transformations:

$$\begin{aligned} z &= 1 - \exp(-\nu\rho) \\ w &= \frac{h}{\ln \chi} \ln[1 + \frac{z}{h}(\chi - 1)] \; , \end{aligned} \quad (2.17)$$

where the parameters ν and χ are chosen in such a way to get the most convenient set of ρ_k values. The main difference between the trasformations (2.16) and (2.17) lies in the fact that, when solving the set of differential equations, a boundary condition mut be imposed at $\rho = \rho_{max}$ in the first case, whereas in the second case, the final point in the w–grid corresponds to $\rho = \infty$, and for such a point the usual boundary condition is that the function to be determined is zero. In the calculation

of the A=3 bound state w.f., both the transformations (2.16) and (2.17) produce almost exactly the same results. However, in the study of scattering states, the asymptotic conditions to be satisfied are more easily fulfilled by the transformation (2.17), which will be therefore the one adopted in the next section.

The ground state of the triton has been studied in ref.[1] by means of the PHH approach with the AV14 potential. The system of equations (2.15) has been solved by including up to 12 channels in the expansion (2.6); for the sake of completeness, we have extended the calculations to include all the channels with $\ell_\alpha + L_\alpha \leq 4$ and the results are displayed in table 1. By inspection of the table, one can see that the PHH expansion is rapidly convergent to results which are in complete agreement with those obtained in ref.[3], where a different technique for constructing the w.f. has been used. These circumstances should eliminate any doubt about a still missing small contribution to the binding energy, due to the use of variational bases in both the approaches.

We have also studied the structure of the A=3 systems when three–body forces are included in the Hamiltonian of the system. Therefore, we have implemented the nucleon interaction by adding to the AV14 potential both the Tucson–Melbourne (TM) and the Brazil (BR) three–body potentials, which have been used by different groups [3,17,18] to study the three–nucleon bound state. In these models the numerical choice of the πN form factor cutoff Λ appears to be critical, the choice $\Lambda = 5.8\mu$ (μ is the pion mass) checked in ref.[17], leads to an overbinding of the trinucleon system. Of course, it is possible to consider also other TBI effects, as for example those due to ρ–meson exchanges [19]. In order to compare with the mentioned calculations, as a first choice we have adopted the same Λ value of ref.[17]. The results obtained by including up to 18 channels are shown in table 2, together with the estimates of the Los Alamos group corresponding to a 34 channels configuration space Faddeev (CSF) calculation [17]. The agreement between the two approaches is very satisfactory. Successively, the value of the cutoff parameter Λ has been changed in order to provide a triton binding energy value close to the experimental one. The results are listed in table 4 for the AV14 + TM and AV14 + BR models and correspond to the values $\Lambda = 5.13\mu$ and $\Lambda = 4.99\mu$, respectively. As mentioned in the introduction, it is necessary that the adopted potential models give a satisfactory description of the A=3 bound states, due to the correlation between low energy scattering observables and ground state binding energy, and for this reason the modified values of the Λ parameter previously given will be used in the next section.

Finally, the ^{3}He ground state could easily be calculated with the same TBI terms and with the Coulomb potential. However, it is well known that the Coulomb interaction alone is not able to completely explain the mass difference between ^{3}H and ^{3}He and other CSB terms must be added to the Hamiltonian [18,19]. This problem will no longer be discussed here.

3. N-d scattering below the break–up threshold

The progress in the experimental and theoretical study of N–d interaction processes during the last decade has been noticeable. In particular, N–d elastic scattering and break-up cross sections data are now available over a large range of energies. Accurate results have been also obtained for polarized nucleon and deuteron targets [8]. The theoretical analyses have been done using a variety of techniques and NN potentials [20,21], including three-body forces too [20,22]. Moreover, the treatment of the Coulomb interaction for the pd system has been improved in a satisfactory way [23]. Nevertheless, the interest in this field remains noticeable, first of all because of the possibility of testing models and techniques by comparing the calculated and experimental values for a number of important observables. For such a reason, it is evident the importance of increasing the accuracy both in the experimental and theoretical studies.

The variational approach based on the use of PHH correlated functions can be extended to investigate scattering states and in this section the application to the N–d scattering below the break–up threshold is discussed. Following the pioneering work of Delves [24] for realistic NN interactions, the wave function for a N–d scattering state will be written as

$$\Psi = \Psi_C + \Psi_A \ . \tag{3.1}$$

The first term Ψ_C must be sufficiently flexible to guarantee a detailed description of the "core" of the system, when the particles are close to each other and the mutual interaction is large; Ψ_C goes to zero when the nucleon–deuteron distance r_{Nd} increases. As in the previous section, Ψ_C is the sum of three Faddeev amplitudes which are in turn expanded in terms of the PHH basis functions. The second term Ψ_A of eq.(3.1) has to describe the asymptotic configurations of the system, for large r_{Nd} values, where the nuclear N–d interaction is negligible. In the asymptotic region the w.f. Ψ reduces to Ψ_A, which therefore must be the appropriate asymptotic solution of the Schroedinger equation. Ψ_A can also be decomposed in three Faddeev amplitudes and each one of these is written as a linear combination of the following functions

$$\Omega^{\lambda}_{LSJ}(\mathbf{x}_i,\mathbf{y}_i) = \sum_{l_\alpha=0,2} w_{l_\alpha}(x_i)\mathcal{R}^{\lambda}_{L}(y_i)\times \\ \left\{\left[[Y_{l_\alpha}(\hat{x}_i)s^{jk}_\alpha]_1\otimes s^i\right]_S\otimes Y_L(\hat{y}_i)\right\}_{JJ_z}[t^{jk}_\alpha t^i]_{TT_z} \ . \tag{3.2}$$

In this equation $w_{l_\alpha}(x_i)$ is the deuteron wave function component in the waves with $l_\alpha = 0, 2$; L is the relative angular momentum of the deuteron and the incident nucleon, S is the spin obtained by coupling the spin 1 of the deuteron to the spin 1/2 of the incident nucleon. Therefore, an asymptotic state will be labelled as ${}^{(2S+1)}L_J$ and the corresponding phase shift as δ_{LSJ}.

The functions $\mathcal{R}_L^\lambda(y_i)$ of eq.(3.1) can be taken as the regular (R) and irregular (I) radial solutions of the two–body (N–d) Schroedinger equation without nuclear interaction. The regular solution, denoted as $\mathcal{I}_L(y_i)$, can be written in the form

$$\mathcal{I}_L(y) = \frac{F_L(\eta,\zeta)}{(2L+1)k^L\zeta C_L(\eta)} \ , \tag{3.3}$$

where $\eta = 2Me^2/3\hbar^2 k$ and $\zeta = kr_{Nd}$ are the usual Coulomb parameters, k is related to the center of mass energy $E_{c.m.} = 3\hbar^2k^2/4M$ and $y = (\sqrt{3}/2)r_{Nd}$. The regular Coulomb function F_L and the factors C_L are defined in the standard way and the non–Coulomb case is obtained in the limit $e^2 \to 0$ (see also ref.[25]). The irregular solution, denoted as $\mathcal{K}_L(y_i)$, has the form

$$\mathcal{K}_L(y) = (2L+1)k^{L+1}C_L(\eta)\frac{G_L(\eta,\zeta)}{\zeta} \tag{3.4}$$

where $G_L(\eta,\zeta)$ is the irregular Coulomb function. The function $\mathcal{R}_L^\lambda(y_i)$ of eq.(3.1) is taken equal to $\mathcal{I}_L(y)$ for $\lambda \equiv R$, whereas for $\lambda \equiv I$ it does not coincide with $\mathcal{K}_L(y)$, since this would introduce a singular behaviour at $r_{Nd} = 0$, which should be corrected by the Ψ_C term in eq.(3.1). In order to avoid it, the function $G_L(\eta,\zeta)$ in eq.(3.4) has been replaced by $\widetilde{G}_L(\eta,\zeta)$, which differs from the previous one by a regularizing factor. Of course, the detailed form of such a factor is not of particular relevance, and in conclusion the following simple form will be used

$$\widetilde{G}_L(\eta,\zeta) = (1-\exp^{-\xi r_{Nd}})^{L+1}G_L(\eta,\zeta) \ . \tag{3.5}$$

The trial parameter ξ is determined by requiring that $\widetilde{G}_L$ tends to G_L smoothly and the value $\xi = 0.25\text{fm}^{-1}$ is found to be adequate. With the above definitions, the i–th Faddeev amplitude for the asymptotic wave function is written as

$$\Omega_{LSJ}(\mathbf{x}_i,\mathbf{y}_i) = \Omega^R_{LSJ}(\mathbf{x}_i,\mathbf{y}_i) + \sum_{L'S'} {}^J\widetilde{R}^{SS'}_{LL'}\Omega^I_{L'S'J}(\mathbf{x}_i,\mathbf{y}_i) \ , \tag{3.6}$$

where the matrix elements ${}^J\widetilde{R}^{SS'}_{LL'}$ give the relative weight between the regular and the irregular components. They are closely related to the corresponding reactance matrix ($\Re$–matrix) elements:

$${}^JR^{SS'}_{LL'} = (2L+1)(2L'+1)k^{L+L'+1}C_LC_{L'}\ {}^J\widetilde{R}^{SS'}_{LL'} \ . \tag{3.7}$$

By definition, the eigenvalues of the $\Re$–matrix are $\tan\delta_{LSJ}$.

The internal part Ψ_C of the w.f. (3.1) is decomposed in the three Faddeev amplitudes and each one is expanded in terms of the PHH basis, as it was done for the bound state

$$\psi_C(\mathbf{x}_i,\mathbf{y}_i) = \sum_{\alpha=1}^{N_c} \Phi_\alpha^C(x_i,y_i)\mathcal{Y}_\alpha(jk,i) \tag{3.8a}$$

$$\Phi_\alpha^C(x_i,y_i) = \rho^{\ell_\alpha+L_\alpha} f_\alpha(x_i)\Big[\sum_{K=K_0}^{K_\alpha} u_K^\alpha(\rho)\ {}^{(2)}P_K^{\ell_\alpha,L_\alpha}(\phi_i)\Big]\ , \tag{3.8b}$$

with the conditions $u_K^\alpha(\rho) \to 0$ when $\rho \to \infty$.

The form of the Ψ_A component is given by eqs.(3.2) and (3.6) also at small interparticle distances, therefore the internal function Ψ_C must properly correct, such a Ψ_A behaviour, in that region. For this reason, the partial wave decomposition of Ψ_C (which is truncated when doing calculations) must include, first of all, those channels that are present in the asymptotic state (open channels), but the summation must be extended also to all the other important α–channels compatible with the state to be described. In conclusion, the total wave function corresponding to an asymptotic state ${}^{(2S+1)}L_J$ will be written as

$$\begin{aligned}\Psi_{LSJ} &= \sum_{i=1,3}\left[\Phi_C(\mathbf{x}_i,\mathbf{y}_i) + \Omega_{LSJ}(\mathbf{x}_i,\mathbf{y}_i)\right] \\ &= \sum_{i=1,3}\left[\Phi_C(\mathbf{x}_i,\mathbf{y}_i) + \Omega^R_{LSJ}(\mathbf{x}_i,\mathbf{y}_i) + \sum_{L'S'} {}^J\widetilde{R}^{SS'}_{LL'}\Omega^I_{L'S'J}(\mathbf{x}_i,\mathbf{y}_i)\right]\ . \end{aligned}\tag{3.9}$$

The Hamiltonian connects states with the same parity and total angular momentum J, but with $\Delta L = 0,1,2$. As a consequence, the $\Re$–matrix for $J = 1/2$ is a 2×2 matrix and it is a 3×3 matrix in all the remaining cases. So, for a given J two or three independent functions (3.9) can be built up by different combinations of L and S.

The quantities to be determined in the wave functions (3.9) are the hyperradial functions (see eq.(3.8b)) and the matrix elements ${}^J\widetilde{R}^{SS'}_{JJ'}$. To this aim we will use the Kohn variational principle. This variational principle establishes that, for scattering states, the $\Re$–matrix elements, considered as functionals of the wave function, must be stationary [23] with respect to variations of all the trial parameters. Explicitely, these functionals are given by:

$$[{}^J\widetilde{R}^{SS'}_{LL'}] = {}^J\widetilde{R}^{SS'}_{LL'} - < \Psi_{L'S'J}|\mathcal{L}|\Psi_{LSJ} > \tag{3.10}$$

$$\mathcal{L} = \frac{M}{2\sqrt{3}\hbar^2}(H-E)\ , \tag{3.11}$$

where ${}^J\widetilde{R}^{SS'}_{LL'}$ are the trial parameters of eq.(3.9). With the above definition of the operator $\mathcal{L}$ and using eqs.(3.2–4), we fix the normalizations of the asymptotic states as

$$< \Omega^R_{LSJ}|\mathcal{L}|\Omega^I_{LSJ} > - < \Omega^I_{LSJ}|\mathcal{L}|\Omega^R_{LSJ} >= 1 \ . \tag{3.12}$$

The variation of the diagonal functionals with respect to the hyperradial functions $u^\alpha_K(\rho)$ is first performed. From the condition

$$\delta_u[{}^J\widetilde{R}^{SS}_{LL}] =< \delta_u\Psi_{LSJ}|\mathcal{L}|\Psi_{LSJ} >= 0, \tag{3.13}$$

and using the same procedure as in the case of the Rayleigh–Ritz variational principle for to the bound state, an inhomogeneous set of second order differential equations is obtained:

$$\sum_{\alpha',K'}\Big[A^{\alpha,\alpha'}_{K,K'}(\rho)\frac{d^2}{d\rho^2} + B^{\alpha,\alpha'}_{K,K'}(\rho)\frac{d}{d\rho} + C^{\alpha,\alpha'}_{K,K'}(\rho) + \frac{m}{\hbar^2}E\ N^{\alpha,\alpha'}_{K,K'}(\rho)\Big]u^{\alpha'}_{K'}(\rho) = D^\lambda_{\alpha K}(\rho)\ . \tag{3.14}$$

The coefficients A, B, C, N have the same expression as in the bound state case, and the inhomogeneous term is given by

$$D^\lambda_{\alpha K}(\rho) = \rho^{l_\alpha+L_\alpha}\sum_{ii'} < f_\alpha(x_i)\ {}^{(2)}P^{l_\alpha L_\alpha}_K(\phi_i)\mathcal{Y}_\alpha(jk,i)|\mathcal{L}|\Omega^\lambda_{LSJ}(\mathbf{x}_{i'},\mathbf{y}_{i'}) >_\Omega\ , \tag{3.15}$$

where, the subscript LSJ has been omitted for simplicity. For each asymptotic state ${}^{(2S+1)}L_J$ two different inhomogeneous terms can be constructed in correspondence to the asymptotic Ω^λ_{LSJ} function with $\lambda \equiv R$ or I. Correspondingly, two different sets of hyperradial functions are obtained by solving the system of eqs.(3.14).

Then, in order to get the optimum choice for the matrix elements ${}^J\widetilde{R}^{SS''}_{LL''}$, the diagonal functionals (3.10) are varied with respect to them. This leads to the following set of algebraic equations

$$\sum_{L'',S''} {}^J\widetilde{R}^{SS''}_{LL''}X^{S'S''}_{L'L''} = Y^{SS'}_{LL'}\ , \tag{3.16}$$

with the coefficients X and Y defined as

$$\begin{aligned} X^{S'S''}_{L'L''} &=< \Omega^I_{S'L'J} + \Psi^I_{S'L'J}|\mathcal{L}|\Omega^I_{S''L''J} > \\ Y^{SS'}_{LL'} &= - < \Omega^R_{SLJ} + \Psi^R_{SLJ}|\mathcal{L}|\Omega^I_{S'L'J} > \end{aligned}\ , \tag{3.17}$$

In the latter equations, Ψ^λ_{LSJ} indicates the internal part of the wave function constructed with one of the two solutions of eqs.(3.14), as previously obtained.

It is worth to notice that the variation of the diagonal functionals gives different coupled equations which must be satisfied by the off–diagonal elements of the reactance matrix [26]. However, the corresponding solutions are a first order variational estimates and the last term in eq.(3.10) is, in general, not zero, as it would happen in the case of the exact wave function. A second order estimate for the $\Re$–matrix elements can be obtained by substituting, in the second member of equation (3.10), the first order results. As the reactance matrix is symmetric, the method should provide ${}^J\widetilde{R}^{SS'}_{LL'} = {}^J\widetilde{R}^{S'S}_{L'L}$. The degree of violation of this condition give useful information about the accuracy of the solution.

4. Numerical results

The numerical technique to solve the inhomogeneous linear equations system (3.14) deserves some attention. The relevant point is that the scattering state w.f. (3.1) must carefully describe both the regions of small and medium–large interparticle distances, the asymptotic behaviour having been properly taken into account throught the Ψ_A component. For this reason, it is convenient to use in place of ρ the variable w, defined by the transformation (2.17). By using this new variable, and after replacing the differential operators by finite differences, the system (3.14) is transformed into a set of algebraic linear equations which can be solved by means of standard methods. We have used $N = 40 \div 50$ w–grid points have been used, the last point ($w_N = 1$) corresponds to $\rho = \infty$ and the penultimate w value corresponds to $\rho_{N-1} \approx 65.0\,\mathrm{fm}$.

The first case considered is a zero energy scattering process. In this case, due to centrifugal barrier effects, the reactance matrix is diagonal and two physical states with $L = 0$ can be constructed: the $J = 1/2$ (doublet) and the $J = 3/2$ (quartet) states. The corresponding scattering lenghts are defined as

$$ {}^{(2J+1)}a_{N-d} = -\lim_{k\to 0} \frac{{}^J\widetilde{R}^{JJ}_{00}}{k} \ . \tag{4.1} $$

The first NN interaction considered is the semi–realistic Malfliet and Tjon [27] potential (I–III) acting only in the s–wave. For this potential the " exact" results of the CSF method [28] are available, therefore a meaningful comparison can be done. Our results are ${}^2a_{n-d} = 0.702\,\mathrm{fm}$ and ${}^2a_{p-d} = 0.003\,\mathrm{fm}$ for the doublet state and ${}^4a_{n-d} = 6.442\,\mathrm{fm}$ and ${}^4a_{p-d} = 13.96\,\mathrm{fm}$ for the quartet one. These values are extremely close to those given by the CSF method.

Then we have considered the realistic AV14 and AV14+BR interactions, with the TBI cutoff parameter $\Lambda = 5.8\mu$. The calculated doublet and quartet scattering lengths are reported in table 4 as a function of the number N_c of channels included in the expansion of the w.f., together with the 34–channels CSF results of ref.[20]. The agreement between the two methods is quite satisfactory, and there are only small differences due to the contributions from higher channels not present the CSF approach.

If the value of the cutoff parameter is taken $\Lambda = 4.99\mu$, so as to reproduce the correct triton binding energy, the resulting scattering lengths are again very close to the CSF ones given in ref.[20]. Concerning the comparison between the theoretical predictions and experimental data, here we only mention that for the n–d case the agreement is acceptable, whereas, as it is discussed in ref.[25], one must be very carefull, for the p–d system, when extrapolating to zero energy the experimental phase shifts obtained at not sufficiently low energies.

The numerical analysis has then been extended to elastic Nd scattering states below the deuteron break–up treshold. For scattering energy different from zero, the reactance matrix, with the exception of states having J=1/2, is a symmetric 3×3 matrix. Its six independent parameters are the three eigenvalues ($\tan \delta_{LSJ}$) and the three mixing parameters which are here introduced by adopting the formalism of Seyler [29]. As it was mentioned in section 3, the solution obtained by means of eqs.(3.16) gives different first–order estimates for the off–diagonals elements. However, the second–order estimates, calculated with the help of eq.(3.10) should verify the symmetric condition with an improved accuracy. In order to stress this aspect of the problem, the first– and second–order estimates for the $\Re$–matrix elements, calculated with the AV14 potential, are shown in table 5 in the case $J = 1/2^+$ and a neutron incident energy of 3.0 MeV, The first four rows of the table correspond to a calculation with a number of channels $N_c = 8$ and $M = 3$ hyperradial functions per channel. For the successive four rows $N_c = 8$ and $M = 6$ have been used and the last four rows are obtained with $N_c = 10$ and $M = 6$. By inspection of the table, it can be seen that the second order variational calculation accurately provides a symmetric reactance matrix and the correction given by the mean value of the operator $\mathcal{L}$ goes to zero as the number of hyperradial functions and channels increase. Analogous rates of convergence have been found for all the states studied in the present work.

Accurate experimantal data and systematic phase shifts analyses exist for the pd system [8], for incident proton energy values E_N=1.0, 2.0, 3.0 MeV. We have calculated the scattering states with the above energy values having in mind the two following motivations. First a detailed comparison with the experimental results using realistic interactions (including also three-body terms) and an adequate treatment of the Coulomb repulsion, is of interest to judge the merits of the theoretical underlying model; second, the calculated $\Re$–matrix elements may be useful in the case of future phase shifts analyses of accurate experimental data.

Coming back to our calculation, the phase shifts with $L > 2$ can be disregarded at the energies here considered, so only twenty independent parameters are contained in the cross section, i.e. thirteen phase shifts and seven mixing parameters. The variational estimates of these twenty parameters are displayed in table 6 at three different values of the scattering energy. For sake of completeness, the system nd has also been studied and the results are reported in the table. The contribution from the TBI terms is unimportant in all the states, with the excep-

tion of the J=$1/2^+$, a circumstance already noticed in ref.[22]. The values listed in table 6 correspond to the AV14 potential, but when the AV14+BR predictions differ appreciably from the AV14 ones, they are reported in parentheses in the table. Concerning the number of channels, the value $N_c = 14$ for $J = 1/2^+$ and $N_c = 18$ for $J = 3/2^+$ have been used. For the other J values N_c has been fixed by including all open channels (giving the major contribution) and a few selected close channels which give a minor but appreciable contribution; in any case the total number of channels does never exceed $N_c = 18$. The number of hyperradial functions per channel can vary in the range $M = 3 \div 6$, with enough flexibility in the radial functions to get convergence for all the calculated matrix elements listed.

5. Discussion and conclusions

The study of the scattering processes involving a few strongly interacting particles is a field of large interest, but only in recent times it has been possible to performe accurate numerical calculations of the important related quantities. An emblematic situation is that one involving three nucleons and, in particular, the N–d interaction processes. For this system, the main progress has been realized by the Faddeev method, both in momentum and coordinate representations. A delicate aspect of such an approach is connected with the treatment of the pp Coulomb interaction. As it is well known, the nuclear and Coulomb potentials are expanded in channels with increasing angular momenta and the expansion is enlarged until a satisfactory convergenge for the w.f. of the system and the (part of) potential taken into account is found. However, the expansion in partial waves of the Coulomb interaction is slowly convergent and the problem of the missing contribution must be carefully investigated.

On the other side, the merit of a variational treatment is that even if the w.f. is expandend in channels, the interaction is fully taken into account as no expansion of the potentials is performed. Of course, the variational tecnique must be devised with particular attention in order to reproduce all the relevant details of the investigated structure. This might appear as easy to be satisfy, since the number of trial parameters can be increased and the computational facilities available at present allow to handle quite easily the corresponding numerical problem. However, this is the situation only for rather simple homework interactions and the variational analyses of the bound and scattering states of the three–nucleon system, with realistic interactions, have encountered severe difficulties. One possible solution is to employ adequate expansion basis for the radial dependence of each channel in the w.f. expansion. Since the NN interaction produces strong nucleon–nucleon correlations, it appears to be convenient to introduce sets of basis functions which in somehow take care of these correlations. A choice, investigated with success in the bound state of the A=3 systems, is a correlad harmonic oscillator (CHO) basis [30. However, in order to reproduce an exponential type behaviour characteristic of the large interparticle distances of the bound state w.f. of nuclear systems , a great

number of HO functions is necessary. With respect to this, the use of correlated hyperspherical harmonic basis appears more convenient, and the results obtained in ref.[1] for the bound state and, in the present paper, for elastic scattering states on three nucleons are very satisfactory.

There are a few aspects of interest in the results presented throughout the paper which we wish to point out. First, there are no difficulties in treating the Coulomb interaction for A=3 scattering states, even above the deuteron break–up threshold. The inclusion of TBI terms in the nuclear interaction does not cause additional problems and it is not necessary to increase the number of the w.f. channels. Again the reason lies in the fact that no expansion in partial waves of the TBI is required. Concerning the numerical studies presented for the N–d elastic scattering processes, we have considered one of the available so–called realistic interactions, i.e. the AV14 potential with the Brazil three–body interaction, with a value of the Λ parameter chosen to produce a correct value of the triton binding energy. However, the extension of the variational method based on PHH correlated functions to other forms of local or non local interactions, as for example the Bonn potential, does not present difficulties and could be useful for precise testing of the adopted model. Indeed, the theoretical analyses allow for accurate evaluations of the phase shifts and mixing parameters in the various channels. Moreover, since there is an overall satisfactory agreement between theoretical and experimantal data, future improvements in the accuracy of the experimental data would certainly be of interest.

We would notice finally that the extension of the proposed variational method to scattering states for systems with larger number of particles, in particular A=4, can be easily performed but the corresponding numerical effort strongly increases. Interesting numerical results can, nevetheless, be again obtained.

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Table Captions.

Table 1. Binding energy (B), kinetic energy mean value (T) and S'–, P and D–wave percentages for ^{3}H and ^{3}He in terms of the number of channels N_c. The 26–channels calculations of ref.[3] are reported in the last row for each case.

Table 2. Binding energies in terms of the number of channels N_c for the indicated potential models. The 34–channels CSF calculations of ref.[17] are given in the last row for the sake of comparison.

Table 3. Results for the triton corresponding to $N_c = 18$, for the two potential model indicated. The πN form factor is chosen to fit the experimental binding as is explained in the text.

Table 4. The doublet and quartet scattering lengths as a function of the number of channels N_c. The 34–channel CSF calculations of ref.[20] are given in the last row for each case.

Table 5. First order and second order estimates for the reactance matrix in three different approximations, as explained in the text. The central column correspons to the evaluation of the last term of eq.(3.10) which summed to the first order estimate gives the second order estimate.

Table 6. Phase shifts and mixing parameters in degrees, calculated for the indicated c.m. energies. For each energy the first and second column correspond to the n–d and p–d case, respectively. The nuclear potential is the AV14 and the numbers in parenthesis correspond to the AV14+BR model.

	^{3}H				
N_c	B(MeV)	T(MeV)	$P_{S'}(\%)$	$P_D(\%)$	$P_P(\%)$
8	7.660	45.551	1.128	8.926	0.066
12	7.678	45.645	1.127	8.962	0.076
18	7.683	45.671	1.126	8.965	0.076
ref.[2]	7.684	45.677	1.126	8.968	0.076
	^{3}He				
N_c	B(MeV)	T(MeV)	$P_{S'}(\%)$	$P_D(\%)$	$P_P(\%)$
8	7.010	44.687	1.318	8.890	0.065
12	7.027	44.780	1.315	8.926	0.075
18	7.032	44.797	1.314	8.931	0.075
ref.[2]	7.033	44.812	1.314	8.932	0.075

Table 1.

N_c	AV14+TM B(MeV)	AV14+BR B(MeV)
8	9.241	9.153
10	9.306	9.218
12	9.315	9.225
14	9.325	9.235
CSF	9.32	9.22

Table 2.

Potential	B(MeV)	T(MeV)	$P_{S'}(\%)$	$P_D(\%)$	$P_P(\%)$
AV14+BR	8.481	49.31	0.928	9.547	0.139
AV14+TM	8.480	49.30	0.938	9.255	0.161

Table 3.

N_c	AV14		AV14 + BR	
	$^2a_{nd}$	$^2a_{pd}$	$^2a_{nd}$	$^2a_{pd}$
3				
8	1.211	0.980	0.048	-1.056
10	1.198	0.957	-0.003	-1.139
12	1.196	0.954	-0.010	-1.145
CSF	1.204	0.965	-0.001	-1.136
	$^4a_{nd}$	$^4a_{pd}$	$^4a_{nd}$	$^4a_{pd}$
3	6.383	13.791	6.376	13.830
10	6.382	13.785	6.375	13.825
14	6.381	13.781	6.374	13.820
18	6.380	13.779	6.373	13.819
CSF	6.380	13.764	6.381	13.765

Table 4.

$M(N_c)$	${}^{J}\widetilde{R}^{SS'}_{LL'}$	$1^{\underline{st}} - order$	$< \Psi_{L'S'J} \mid \mathcal{L} \mid \Psi_{LSJ} >$	$2^{\underline{nd}} - order$
3(8)	${}^{1/2}\widetilde{R}^{\frac{1}{2}\frac{1}{2}}_{00}$	2.778	-0.003	2.775
	${}^{1/2}\widetilde{R}^{\frac{1}{2}\frac{3}{2}}_{02}$	0.821	0.028	0.849
	${}^{1/2}\widetilde{R}^{\frac{3}{2}\frac{1}{2}}_{20}$	0.850	-0.001	0.849
	${}^{1/2}\widetilde{R}^{\frac{3}{2}\frac{3}{2}}_{22}$	62.07	3.665	65.74
6(8)	${}^{1/2}\widetilde{R}^{\frac{1}{2}\frac{1}{2}}_{00}$	2.753	0.002	2.755
	${}^{1/2}\widetilde{R}^{\frac{1}{2}\frac{3}{2}}_{02}$	0.857	-0.008	0.849
	${}^{1/2}\widetilde{R}^{\frac{3}{2}\frac{1}{2}}_{20}$	0.847	0.002	0.849
	${}^{1/2}\widetilde{R}^{\frac{3}{2}\frac{3}{2}}_{22}$	65.84	0.316	65.52
6(10)	${}^{1/2}\widetilde{R}^{\frac{1}{2}\frac{1}{2}}_{00}$	2.746	0.001	2.747
	${}^{1/2}\widetilde{R}^{\frac{1}{2}\frac{3}{2}}_{02}$	0.854	-0.009	0.845
	${}^{1/2}\widetilde{R}^{\frac{3}{2}\frac{1}{2}}_{20}$	0.845	0.000	0.845
	${}^{1/2}\widetilde{R}^{\frac{3}{2}\frac{3}{2}}_{22}$	65.88	-0.416	65.46

Table 5.

$E_{c.m.}$(MeV)	0.667		1.333		2.0	
	n–d	p–d	n–d	p–d	n–d	p–d
$^2S_{1/2}$	-17.7	-12.6	-27.9	-23.6	-34.9	-31.4
	(-14.5)	(-9.54)	(-24.0)	(-19.8)	(-30.6)	(-27.3)
$^4D_{1/2}$	-1.00	-0.79	-2.58	-2.28	-3.91	-3.62
	(-1.00)	(-0.78)	(-2.57)	(-2.28)	(-3.90)	(-3.61)
$\eta_{1/2}$	1.04	1.19	1.21	1.25	1.26	1.26
	(1.50)	(1.85)	(1.60)	(1.73)	(1.61)	(1.67)
$^4S_{3/2}$	-47.2	-37.4	-61.3	-53.5	-70.5	-63.7
$^2D_{3/2}$	0.60	0.45	1.55	1.36	2.42	2.20
$^4D_{3/2}$	-1.08	-0.84	-2.77	-2.46	-4.22	-3.91
$\varepsilon_{3/2}$	0.65	0.83	0.72	0.79	0.78	0.84
$\zeta_{3/2}$	-0.11	-0.09	-0.23	-0.20	-0.37	-0.32
$\eta_{3/2}$	0.55	0.53	1.01	0.98	1.44	1.39
$^2D_{5/2}$	0.57	0.45	1.53	1.34	2.38	2.17
$^4D_{5/2}$	-1.14	-0.91	-2.98	-2.64	-4.57	-4.23
$\varepsilon_{5/2}$	-0.29	-0.37	-0.30	-0.34	-0.31	-0.35
$^4D_{7/2}$	-1.06	-0.84	-2.73	-2.42	-4.15	-3.84
$^2P_{1/2}$	-4.54	-3.61	-7.66	-6.83	-9.51	-8.85
$^4P_{1/2}$	12.2	9.30	19.9	17.5	23.9	22.0
$\varepsilon_{1/2}$	2.92	2.51	3.95	3.48	5.75	4.46
$^2P_{3/2}$	-4.51	-3.58	-7.57	-6.76	-9.34	-8.72
$^4P_{3/2}$	14.2	10.9	22.6	20.0	26.2	24.5
$\varepsilon_{3/2}$	-1.02	-0.86	-1.45	-1.25	-1.91	-1.67
$^4P_{5/2}$	13.2	10.1	21.5	18.9	25.6	23.6

Table 6.